Investigating electronic properties in the semiconductor crystal zinc telluride (ZnTe)

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Abstract

In this article, structural and electronic properties which including the equilibrium lattice parameter (a), bulk modulus (B) , the pressure derivative of the bulk modulus (B'),,volume compressibility(K_V) and band structure in semiconductor crystal ZnTe in the cubic phase are investigated. The calculations have been performed using plane wave sets with pseudopotential in framework of density functional theory(DFT) with various generalized gradient approximations (GGA) and local density approximations (LDA), using PWscf package.Acquired results prove that the energy bands do not cut the Fermi level, So ZnTe is a semiconductor. This compound has a direct band gap 2.35(eV) in Γ point. This is highly excellent agreed with experimental results. It can be concluded that the spin does not effect on these calculations.

Keywords; ZnTe, Zinc blende structure, Band structure, Electronic properties

INTRODUCTION

ZnTe is a direct transition compound semiconductor whose bandgap is 2.26 eV. ZnTe is belonged to a family of (IIB–VIA) compounds. This compound is crystallized in different structural phases such as in cubic zinc blende structure with lattice constant a=6.1030A [1]. Conclusive experimental and theoretical results in ZnTe have recently confirmed the sequence zinc blende$\rightarrow$cinnabar $\rightarrow$ Cmcm, although the presence of a rocksalt structure after Cmcm remains unclear[2-4]. From a theoretical point of view, on Elastic, electronic and structural properties, a several first principles calculations were made for ZnTe composition by a variety of methods including full-potential linear augmented plane-wave method plus local orbitals (FP-APW + lo), tight binding linear muffin tin orbital method (TB-LMTO) and LDA+U approach[1,5,6]. This compound is primarily candidated for semiconductor devices, lasers diodes, macro wave generators, solar cells as the substrate layer and green LED materials etc[7]. Figure (1) shows the Conventional unit cell of zinc blende structure of this composition.

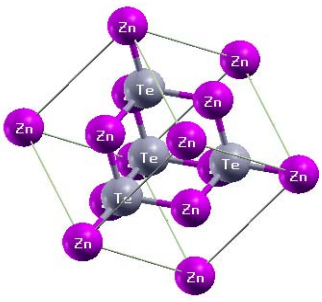

FIG. 1.Conventional unit cell of the zinc-blende Structure[XCrySDen].

METHOD

The calculations have been performed using plane wave sets with pseudopotential in framework of (DFT) with various generalized gradient approximations (GGA) and local density approximations (LDA), using PWscf package. In this research, for making pseudopotential elements Zn and Te, we select the norm conserving pseudopotential method and that is cause of using the homogeneous gas approximation (LDA) and energy exchange correlation (VWN). The cutoff kinetic energy for the plane-wave basis wave functions is chosen as 35 Ry for the calculations. By testing the obtained pseudopotential in different configurations and compare with real calculations, the obtained error is about 10^{-7} Ry. The convergence is based on energy that for the zinc blende structure. We get convergence with 7 iteration and 5.5×10^{-7} Ry estimate. The Monkhorst-Pack k-point mesh of 3×3×3 for the zinc blende structure was employed.

RESULTS AND DISCUSSION

One of the important parameters in these calculations is the lattice constant. This constant is measured experimentally and available, however, theoretical issue must be calculated for confirming. we optimize some of parameters such as the cutoff kinetic energy and the k-point mesh that obtian for the zinc blende structure 35 Ry purposely. The energy variations were obtained through the murnaghan equation of state. By using this equation, the minimum energy of ZnTe in various approximations and through calculated the parameters was obtained. After calculating, the other quantities such as lattice constant, bulk moduli (B), the pressure derivative of the bulk modulus (B') and volume compressibility(K_V) of zinc blende structure in generalized gradient approximations (GGA) and local density approximations (LDA). In Table 1, we summarized our calculated (a), (B),(B') and(K_V) for the zinc blende ZnTe,in comparison with the experimental data and previous theoretical calculations.

Table .1.Calculated lattice constant (in A °), bulk modulus (in GPa), pressure derivative (B') and volume compressibility(K_V) at equilibrium volume in zinc blende structure for ZnTe compound compared to experimental and other theoretical works.

Calculation type	Present work		Other work			
structural parameter	without considering spin polarization	considering spin polarization	Theoretical[1]	Theoretical[8]	Theoretical[9]	Experimental[10]
a(Å)	6.200	6.200	6.00	6.174	6.002	6.103
difference percent comparison with experimental values	1.6%	1.6%	1.7%	1.2%	1.65%	----
B(GPa)	48.63	48.63	55.21	51.2	55.4	50.9
difference percent comparison with experimental values	3.7%	3.7%	9.3%	1.4%	9.7%	----
B'	5.40	5.40	4.60	4.88	---	5
$K_V(GPa)^{-1}$	2.05×10^{-2}	2.05×10^{-2}	1.81×10^{-2}	---	1.80×10^{-2}	2.05×10^{-2}
difference percent comparison with experimental values	3.5%	3.5%	8.5%	---	8.83%	---

Our calculated values are highly excellent agreed with available theoretical and experimental results. By comparison of obtained values for the lattice constant , structural parameters and volume compressibility in the table (1), we realize that the considering spin polarization and without considering spin polarization does not effect on calculations. This shows that the ZnTe is a non-magnetic compound.

By calculating energy band structure, the properties of compound can be found. Fig. 2, shows the calculated band structure at equilibrium volume along high symmetry directions for zinc blende structure ZnTe. In this figure, the fermi energy is selected as the origin and energy scale is according to the electron volt. In Fig. 2, the variation of energy of ZnTe with respect to the electronic wave vectors is drawn.

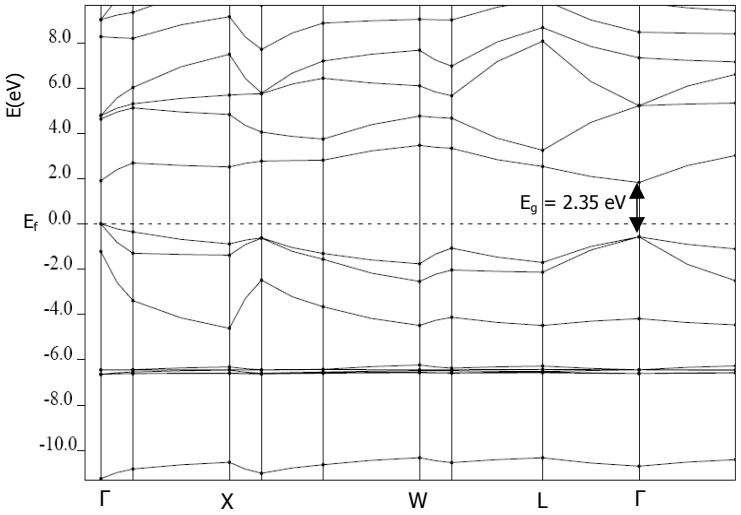

FIG. 2. Band structure along high symmetry directions for zinc blende structure ZnTe.

In this figure, the valence band maximum (VBM) and conduction band minimum (CBM) are occur at the Γ point. Thus, the energy gap is directed between the top of the valence band and the bottom of conduction band at Γ point. The comparison of the band gap with experimental results and existing theoretical calculations are reported in Table 2.

Calculation type / structural parameter	Present work		Other work				
	without considering spin polarization	considering spin polarization	Theoretical[1]	Theoretical[11]	Theoretical[9]	Theoretical[12]	Experimental[13]
Eg (eV)	2.35	2.35	1.28	2.6	1.30	1.33	2.39
Gap type in Γ point	Direct gap	Direct gap	Direct gap	Direct gap	Direct gap	Direct gap	Direct gap
difference percent comparison with experimental values	1.6%	1.6%	46.4%	8.7%	45.6%	44.3%	--

Table.2. Band gaps (eV) from ZnTe in zinc blende structure[1].

It can be concluded that the spin does not effect on energy band structure in this compound. Calculated energy gap with pseudopotential method is highly excellent agreed with experimental results.

CONCLUSION

The calculations have been performed using plane wave sets with pseudopotential in framework of (DFT). Energy band structure of ZnTe in zinc blende structure shows that there is a direct gap in2.35eV in Γ point. This shows that the ZnTe is a semiconductor compound. This results is highly excellent agreed with available experimental and theoretical results. Considering spin polarization does not effect on alculations too. This shows that the ZnTe is a non-magnetic compound.

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